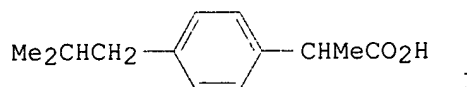


L3 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:125100 CAPLUS
DOCUMENT NUMBER: 102:125100
TITLE: Conformational analysis of some α -phenylpropionic acids with anti-inflammatory activity
AUTHOR(S): Smeyers, Y. G.; Cuellare-Rodriguez, S.; Galvez-Ruano, E.; Arias-Perez, M. S.
CORPORATE SOURCE: Inst. Estruct. Mater., CSIC, Madrid, Spain
SOURCE: Journal of Pharmaceutical Sciences (1985), 74(1), 47-9
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB CNDO/2 quantum mech. conformational calcns., as well as ^{13}C and ^1H NMR measurements, were carried out for the propionic acid residues of 2-(p-isobutylphenyl)propionic acid ibuprofen (I) [15687-27-1] and 2-methyl-2-(p-isobutylphenyl)propionic acid [95499-72-2]. A relationship between the conformational angle of the propionic acid residue and the anti-inflammatory activity appears to exist. The more open the Ph- $\text{C}\alpha$ -COOH dihedral angle, the larger the anti-inflammatory activity.

IT 95499-72-2
RL: PRP (Properties)
(conformation of, anti-inflammatory activity in relation to)

RN 95499-72-2 CAPLUS
CN Benzeneacetic acid, α,α -dimethyl-4-(2-methylpropyl)- (9CI)
(CA INDEX NAME)

